



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:17 PM GMT

PDB ID : 1LTD  
Title : THE 2.6 ANGSTROMS REFINED STRUCTURE OF THE ESCHERICHIA COLI RECOMBINANT SACCHAROMYCES CEREVISIAE FLAVOCYTOCHROME B2-SULPHITE COMPLEX  
Authors : Tegoni, M.; Cambillau, C.  
Deposited on : 1994-01-14  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

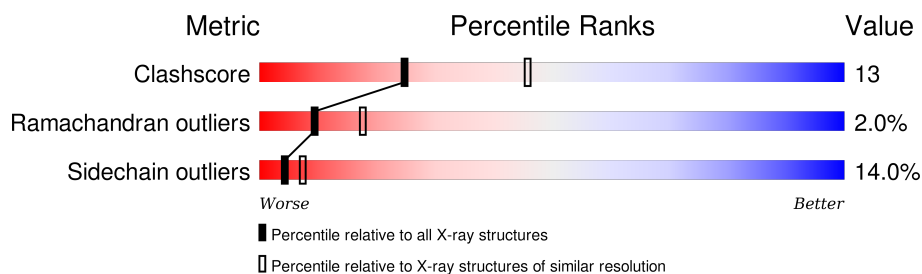
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	506	
1	B	506	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FMN	A	570	X	-	-	-
3	FMN	B	570	X	-	-	-

## 2 Entry composition [i](#)

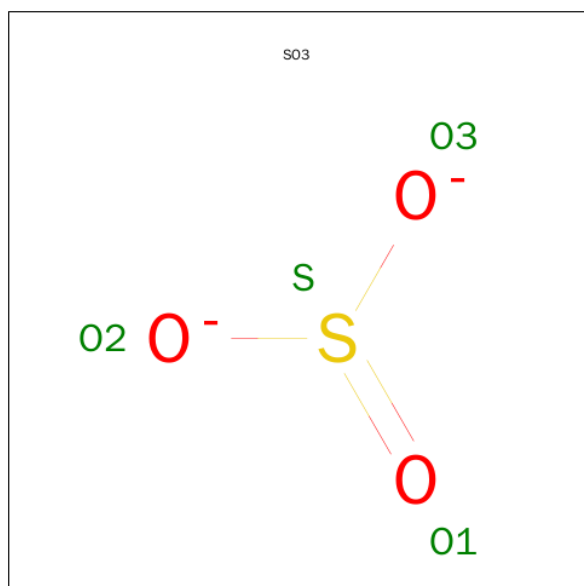
There are 5 unique types of molecules in this entry. The entry contains 7075 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called FLAVOCYTOCHROME B2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	1
			3742	2386	633	709	14			
1	B	387	Total	C	N	O	S	0	0	1
			3014	1913	513	577	11			

- Molecule 2 is SULFITE ION (three-letter code: SO3) (formula: O<sub>3</sub>S).



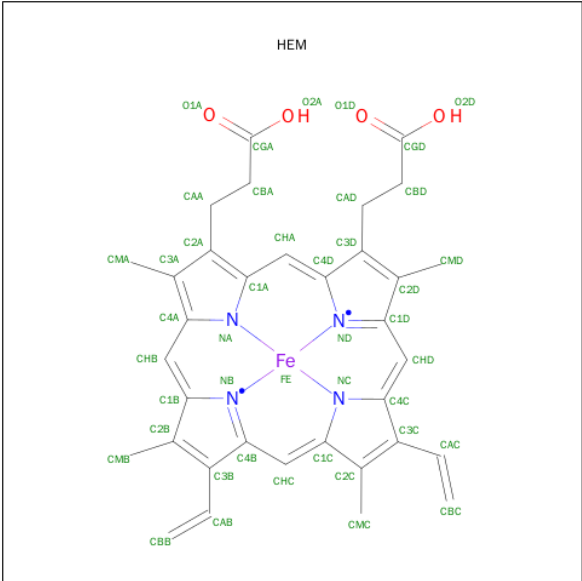
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			4	3	1		
2	B	1	Total	O	S	0	0
			4	3	1		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 5 is water.

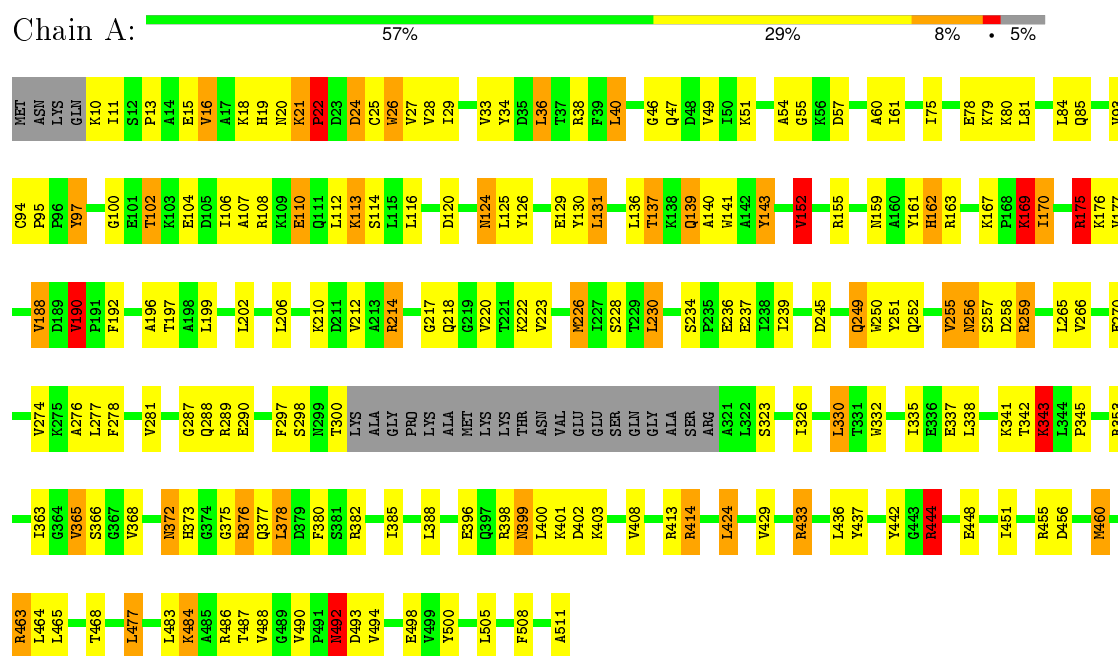
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	145	Total 145	O 145	0	0
5	B	61	Total 61	O 61	0	0

### 3 Residue-property plots

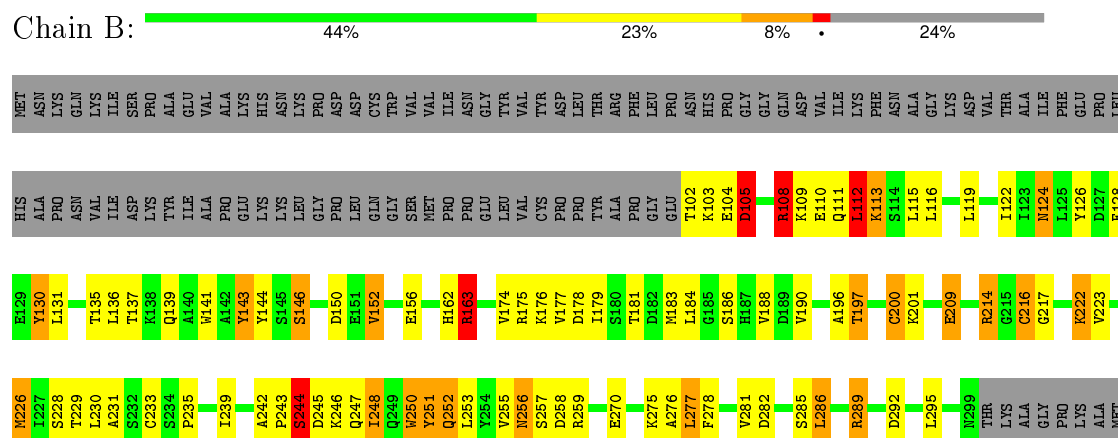
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

#### • Molecule 1: FLAVOCYTOCHROME B2



#### • Molecule 1: FLAVOCYTOCHROME B2





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	164.50 Å   164.50 Å   114.00 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	6.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.60)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.173 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7075	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, HEM, SO3

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.99	0/3816	1.86	80/5170 (1.5%)
1	B	1.00	0/3063	1.83	59/4138 (1.4%)
All	All	0.99	0/6879	1.84	139/9308 (1.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
All	All	0	4

There are no bond length outliers.

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	376	ARG	NE-CZ-NH1	19.71	130.16	120.30
1	A	382	ARG	NE-CZ-NH2	-18.40	111.10	120.30
1	B	463	ARG	NE-CZ-NH2	-15.52	112.54	120.30
1	A	486	ARG	NE-CZ-NH2	-14.28	113.16	120.30
1	A	376	ARG	NE-CZ-NH2	-13.88	113.36	120.30
1	A	486	ARG	NE-CZ-NH1	13.79	127.19	120.30
1	B	382	ARG	NE-CZ-NH2	-13.06	113.77	120.30
1	B	486	ARG	NE-CZ-NH1	12.66	126.63	120.30
1	B	251	TYR	CB-CG-CD1	-11.68	113.99	121.00
1	A	433	ARG	NE-CZ-NH1	11.39	125.99	120.30
1	B	353	ARG	NE-CZ-NH1	11.24	125.92	120.30
1	B	163	ARG	NE-CZ-NH1	11.19	125.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	414	ARG	NE-CZ-NH1	11.12	125.86	120.30
1	A	414	ARG	NE-CZ-NH2	-11.00	114.80	120.30
1	B	143	TYR	CB-CG-CD1	-10.30	114.82	121.00
1	B	382	ARG	NE-CZ-NH1	9.79	125.19	120.30
1	A	226	MET	CG-SD-CE	-9.75	84.60	100.20
1	B	353	ARG	NE-CZ-NH2	-9.57	115.52	120.30
1	B	108	ARG	NE-CZ-NH1	9.37	124.98	120.30
1	A	214	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	A	175	ARG	NE-CZ-NH1	9.19	124.89	120.30
1	A	289	ARG	NE-CZ-NH2	-9.08	115.76	120.30
1	A	289	ARG	NE-CZ-NH1	8.97	124.79	120.30
1	B	463	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	B	368	VAL	CA-CB-CG2	-8.64	97.95	110.90
1	A	492	ASN	CA-C-N	-8.57	98.34	117.20
1	A	382	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	B	226	MET	CG-SD-CE	-8.29	86.94	100.20
1	B	108	ARG	NE-CZ-NH2	-8.09	116.26	120.30
1	B	332	TRP	CD1-CG-CD2	7.96	112.67	106.30
1	A	112	LEU	CA-CB-CG	7.95	133.59	115.30
1	B	250	TRP	CD1-CG-CD2	7.95	112.66	106.30
1	A	332	TRP	CD1-CG-CD2	7.94	112.65	106.30
1	B	413	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	B	141	TRP	CD1-CG-CD2	7.92	112.63	106.30
1	B	376	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	A	250	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	A	214	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	B	444	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	B	251	TYR	CB-CG-CD2	7.63	125.58	121.00
1	A	26	TRP	CD1-CG-CD2	7.63	112.41	106.30
1	B	332	TRP	CE2-CD2-CG	-7.57	101.24	107.30
1	B	141	TRP	CE2-CD2-CG	-7.49	101.31	107.30
1	B	437	TYR	CB-CG-CD2	-7.49	116.51	121.00
1	A	353	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	B	444	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	A	136	LEU	CA-CB-CG	7.24	131.96	115.30
1	A	332	TRP	CE2-CD2-CG	-7.17	101.56	107.30
1	B	250	TRP	CE2-CD2-CG	-7.17	101.57	107.30
1	A	433	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	B	141	TRP	CG-CD2-CE3	6.90	140.11	133.90
1	A	493	ASP	N-CA-CB	-6.86	98.25	110.60
1	A	141	TRP	CE2-CD2-CG	-6.81	101.85	107.30
1	A	97	TYR	CB-CG-CD2	-6.80	116.92	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	490	VAL	CG1-CB-CG2	-6.77	100.07	110.90
1	A	155	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	141	TRP	NE1-CE2-CZ2	-6.66	123.07	130.40
1	A	143	TYR	CB-CG-CD2	-6.64	117.02	121.00
1	A	413	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	A	444	ARG	CG-CD-NE	-6.55	98.05	111.80
1	A	230	LEU	CB-CG-CD2	-6.54	99.89	111.00
1	A	26	TRP	CE2-CD2-CG	-6.52	102.08	107.30
1	A	274	VAL	CG1-CB-CG2	6.50	121.31	110.90
1	A	190	VAL	N-CA-CB	-6.47	97.25	111.50
1	A	259	ARG	NE-CZ-NH2	-6.45	117.07	120.30
1	B	216	CYS	CA-CB-SG	-6.34	102.58	114.00
1	B	112	LEU	CA-CB-CG	6.33	129.87	115.30
1	B	289	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	B	508	PHE	N-CA-CB	6.22	121.79	110.60
1	A	188	VAL	CG1-CB-CG2	-6.17	101.02	110.90
1	B	141	TRP	CB-CG-CD1	-6.15	119.01	127.00
1	A	113	LYS	CA-C-N	-6.15	103.68	117.20
1	A	40	LEU	CA-CB-CG	6.14	129.42	115.30
1	A	297	PHE	CB-CG-CD2	-6.04	116.57	120.80
1	A	220	VAL	CG1-CB-CG2	-6.04	101.23	110.90
1	A	250	TRP	CE2-CD2-CG	-6.04	102.47	107.30
1	A	190	VAL	CG1-CB-CG2	6.00	120.51	110.90
1	A	378	LEU	CB-CG-CD1	-5.98	100.83	111.00
1	B	507	GLU	N-CA-C	5.98	127.15	111.00
1	B	455	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	A	155	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	A	408	VAL	CG1-CB-CG2	-5.95	101.38	110.90
1	B	244	SER	N-CA-C	5.90	126.94	111.00
1	A	108	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	B	368	VAL	CA-CB-CG1	5.82	119.63	110.90
1	A	342	THR	CA-CB-CG2	5.80	120.52	112.40
1	A	141	TRP	CD1-CG-CD2	5.73	110.88	106.30
1	B	130	TYR	CB-CG-CD2	-5.72	117.57	121.00
1	B	408	VAL	O-C-N	-5.72	113.55	122.70
1	A	492	ASN	O-C-N	5.65	131.73	122.70
1	A	251	TYR	CB-CG-CD1	-5.63	117.62	121.00
1	B	483	LEU	CB-CG-CD1	-5.62	101.45	111.00
1	B	188	VAL	CG1-CB-CG2	-5.59	101.96	110.90
1	A	34	TYR	CB-CG-CD1	-5.56	117.66	121.00
1	A	167	LYS	CB-CG-CD	-5.55	97.18	111.60
1	B	286	LEU	CA-CB-CG	5.53	128.03	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	ILE	N-CA-C	-5.53	96.06	111.00
1	B	181	THR	N-CA-C	-5.49	96.18	111.00
1	B	259	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	161	TYR	CB-CG-CD1	-5.43	117.74	121.00
1	B	362	GLU	CA-CB-CG	-5.43	101.45	113.40
1	B	250	TRP	CG-CD2-CE3	5.41	138.77	133.90
1	B	455	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	332	TRP	CG-CD1-NE1	-5.41	104.69	110.10
1	B	410	GLY	CA-C-N	-5.39	105.42	116.20
1	B	197	THR	N-CA-CB	-5.37	100.10	110.30
1	A	365	VAL	N-CA-CB	-5.35	99.72	111.50
1	A	442	TYR	CB-CG-CD2	-5.34	117.80	121.00
1	A	330	LEU	CA-CB-CG	5.32	127.54	115.30
1	A	455	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	A	108	ARG	CB-CG-CD	-5.29	97.85	111.60
1	A	398	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	152	VAL	CA-C-N	5.27	128.79	117.20
1	A	250	TRP	CG-CD1-NE1	-5.27	104.83	110.10
1	B	200	CYS	CB-CA-C	-5.26	99.89	110.40
1	A	332	TRP	CG-CD2-CE3	5.25	138.63	133.90
1	B	362	GLU	CA-C-N	5.25	128.75	117.20
1	B	378	LEU	CB-CA-C	-5.21	100.30	110.20
1	A	152	VAL	CG1-CB-CG2	5.18	119.20	110.90
1	B	184	LEU	CA-CB-CG	5.18	127.22	115.30
1	A	378	LEU	CA-CB-CG	5.17	127.18	115.30
1	A	343	LYS	CA-CB-CG	5.15	124.72	113.40
1	A	169	LYS	CB-CA-C	-5.14	100.11	110.40
1	A	29	ILE	CA-CB-CG2	-5.13	100.64	110.90
1	A	230	LEU	CA-CB-CG	5.13	127.10	115.30
1	B	113	LYS	CA-C-N	-5.13	105.92	117.20
1	B	414	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	214	ARG	CA-CB-CG	-5.11	102.15	113.40
1	B	418	VAL	CG1-CB-CG2	-5.11	102.72	110.90
1	A	80	LYS	N-CA-C	-5.08	97.27	111.00
1	A	26	TRP	CG-CD1-NE1	-5.07	105.03	110.10
1	A	500	TYR	CB-CG-CD1	5.06	124.03	121.00
1	A	259	ARG	CG-CD-NE	-5.05	101.19	111.80
1	A	484	LYS	O-C-N	-5.05	114.61	122.70
1	B	353	ARG	CA-C-N	5.05	128.32	117.20
1	A	249	GLN	CA-CB-CG	-5.04	102.30	113.40
1	A	281	VAL	CA-CB-CG1	-5.03	103.36	110.90
1	A	424	LEU	CA-C-N	5.03	126.25	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	332	TRP	CG-CD1-NE1	-5.03	105.07	110.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	130	TYR	Sidechain
1	A	463	ARG	Sidechain
1	A	492	ASN	Mainchain
1	B	251	TYR	Sidechain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3742	0	3794	98	0
1	B	3014	0	3072	94	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	31	0	18	1	0
3	B	31	0	17	1	0
4	A	43	0	30	5	0
5	A	145	0	0	2	0
5	B	61	0	0	2	0
All	All	7075	0	6931	177	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (177) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:VAL:HG22	1:B:490:VAL:HG21	1.49	0.95
1:A:199:LEU:HD21	4:A:560:HEM:HAA1	1.71	0.72
1:A:372:ASN:HD22	1:A:375:GLY:H	1.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:VAL:HG22	1:B:490:VAL:CG2	2.19	0.71
1:B:243:PRO:HD2	1:B:247:GLN:HE22	1.55	0.71
1:A:256:ASN:HD22	1:A:257:SER:N	1.88	0.71
1:A:396:GLU:HG3	1:A:401:LYS:HG3	1.75	0.69
1:B:197:THR:HG21	1:B:436:LEU:HG	1.73	0.69
1:A:61:ILE:HD12	1:A:97:TYR:HB2	1.75	0.68
1:A:137:THR:HG22	1:A:140:ALA:H	1.59	0.67
1:B:217:GLY:HA3	1:B:247:GLN:NE2	2.09	0.66
1:A:177:VAL:HG23	1:A:468:THR:HA	1.79	0.65
1:A:190:VAL:HG11	1:A:223:VAL:HG22	1.77	0.65
1:A:162:HIS:HE1	5:A:674:HOH:O	1.80	0.64
1:A:116:LEU:HD22	1:A:131:LEU:HG	1.80	0.64
1:B:109:LYS:HD2	1:B:112:LEU:HD21	1.79	0.63
1:A:511:ALA:H	1:B:115:LEU:HD13	1.63	0.63
1:A:25:CYS:SG	1:A:54:ALA:HB2	2.39	0.63
1:A:385:ILE:HD11	1:A:424:LEU:HD12	1.80	0.63
1:B:256:ASN:HD22	1:B:257:SER:N	1.97	0.62
1:A:27:VAL:HG11	1:A:36:LEU:HD22	1.81	0.62
1:A:28:VAL:HG22	1:A:33:VAL:HG22	1.81	0.62
1:B:216:CYS:O	1:B:222:LYS:HA	2.00	0.61
1:B:105:ASP:O	1:B:109:LYS:HG2	2.00	0.61
1:B:353:ARG:HD2	1:B:355:GLU:HB2	1.81	0.61
1:B:163:ARG:NH2	1:B:486:ARG:HG3	2.16	0.60
1:A:143:TYR:O	1:A:376:ARG:NH2	2.33	0.60
1:A:337:GLU:O	1:A:341:LYS:HD3	2.02	0.60
1:B:354:THR:HA	1:B:391:THR:HG22	1.85	0.59
1:A:270:GLU:OE2	1:A:343:LYS:HG3	2.02	0.59
1:A:414:ARG:HD2	1:B:150:ASP:OD2	2.02	0.59
1:A:266:VAL:HG13	1:A:277:LEU:HD11	1.85	0.59
1:A:463:ARG:HD2	1:B:285:SER:OG	2.02	0.59
1:A:396:GLU:HA	1:A:401:LYS:HB2	1.86	0.57
1:B:109:LYS:HA	1:B:112:LEU:HD23	1.87	0.57
1:A:169:LYS:HG2	1:A:465:LEU:O	2.05	0.56
1:A:170:ILE:HD11	1:B:282:ASP:HA	1.88	0.56
1:A:196:ALA:HB1	1:A:228:SER:HB2	1.88	0.56
1:A:465:LEU:HD23	1:B:378:LEU:HD11	1.88	0.56
1:B:256:ASN:ND2	1:B:258:ASP:H	2.05	0.55
1:A:176:LYS:HA	5:A:661:HOH:O	2.07	0.55
1:B:177:VAL:HG22	1:B:468:THR:HA	1.88	0.55
1:B:152:VAL:HG21	1:B:380:PHE:CE1	2.41	0.55
1:B:256:ASN:HD22	1:B:257:SER:H	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:VAL:HA	1:A:26:TRP:HE3	1.73	0.54
1:A:287:GLY:H	1:A:377:GLN:NE2	2.05	0.54
1:A:163:ARG:NH1	1:B:488:VAL:O	2.41	0.54
1:A:196:ALA:H	1:A:226:MET:HE1	1.72	0.54
1:A:57:ASP:HB3	1:A:93:VAL:HG12	1.88	0.54
1:A:217:GLY:O	1:A:222:LYS:NZ	2.41	0.54
1:A:372:ASN:ND2	1:A:375:GLY:H	2.06	0.53
1:B:369:VAL:HG22	1:B:407:PHE:HB2	1.91	0.53
1:A:218:GLN:HE22	1:A:444:ARG:HD3	1.73	0.53
1:B:404:LEU:HD12	1:B:405:GLU:O	2.07	0.53
1:B:354:THR:OG1	1:B:391:THR:HG22	2.09	0.53
1:A:152:VAL:HG21	1:A:380:PHE:CE1	2.44	0.53
1:A:511:ALA:N	1:B:115:LEU:HD13	2.23	0.53
1:A:223:VAL:HG21	1:A:451:ILE:HG12	1.91	0.52
1:A:197:THR:HB	1:A:436:LEU:HD11	1.90	0.52
1:A:169:LYS:HA	1:B:353:ARG:HH21	1.74	0.52
1:B:375:GLY:HA2	5:B:767:HOH:O	2.10	0.52
1:A:196:ALA:HB2	1:A:226:MET:HE2	1.92	0.52
1:B:452:GLU:HB3	1:B:455:ARG:NH2	2.24	0.52
1:B:394:ILE:HD13	1:B:397:GLN:HE22	1.75	0.52
1:B:183:MET:HE2	1:B:250:TRP:HH2	1.74	0.52
1:B:465:LEU:HD22	1:B:477:LEU:HG	1.92	0.52
1:A:60:ALA:HB3	1:A:94:CYS:O	2.10	0.52
1:A:49:VAL:HB	4:A:560:HEM:HBC2	1.92	0.51
1:A:456:ASP:O	1:A:460:MET:HB2	2.10	0.51
1:A:16:VAL:HA	1:A:26:TRP:CE3	2.45	0.51
1:B:289:ARG:HD2	5:B:764:HOH:O	2.10	0.51
1:B:373:HIS:O	1:B:376:ARG:HG3	2.11	0.51
1:B:243:PRO:HD2	1:B:247:GLN:NE2	2.24	0.51
1:A:508:PHE:HE2	1:B:116:LEU:HD23	1.75	0.51
1:B:270:GLU:OE2	1:B:343:LYS:HB3	2.11	0.51
1:B:143:TYR:O	1:B:376:ARG:NH2	2.42	0.51
1:B:209:GLU:HG3	1:B:231:ALA:HB1	1.93	0.51
1:A:210:LYS:O	1:A:214:ARG:HG3	2.10	0.50
1:B:252:GLN:HA	1:B:278:PHE:O	2.11	0.50
1:A:140:ALA:HB2	1:A:202:LEU:HB3	1.92	0.50
1:A:373:HIS:O	1:A:376:ARG:HG3	2.12	0.50
1:A:15:GLU:O	1:A:18:LYS:HB2	2.12	0.50
1:B:108:ARG:O	1:B:111:GLN:HB2	2.12	0.50
1:A:124:ASN:ND2	1:A:126:TYR:HB2	2.27	0.49
1:A:256:ASN:ND2	1:A:258:ASP:H	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:TYR:O	1:B:433:ARG:HD3	2.12	0.49
1:B:235:PRO:O	1:B:239:ILE:HG13	2.13	0.49
1:B:216:CYS:HB3	1:B:223:VAL:O	2.12	0.49
1:A:252:GLN:HA	1:A:278:PHE:O	2.13	0.49
1:B:179:ILE:HG22	1:B:462:MET:SD	2.53	0.48
1:A:487:THR:O	1:B:490:VAL:HG22	2.14	0.48
1:A:61:ILE:CD1	1:A:97:TYR:HB2	2.43	0.48
1:A:400:LEU:O	1:A:403:LYS:HG2	2.14	0.48
1:A:234:SER:OG	1:A:237:GLU:HG3	2.14	0.48
1:A:494:VAL:O	1:A:498:GLU:HB2	2.13	0.48
1:A:288:GLN:HE21	1:A:290:GLU:HG2	1.78	0.48
1:A:169:LYS:HB3	1:B:353:ARG:NH2	2.29	0.47
1:A:505:LEU:HD13	1:B:130:TYR:HB2	1.96	0.47
1:A:100:GLY:H	1:A:300:THR:N	2.11	0.47
1:B:419:LEU:HD13	1:B:465:LEU:HD12	1.95	0.47
1:B:109:LYS:O	1:B:113:LYS:HB3	2.15	0.47
1:B:108:ARG:HH21	1:B:137:THR:HA	1.80	0.47
1:B:174:VAL:O	1:B:463:ARG:HD2	2.14	0.47
1:A:170:ILE:HG12	1:B:281:VAL:HG23	1.96	0.46
1:A:363:ILE:HG21	1:A:363:ILE:HD13	1.67	0.46
1:A:169:LYS:HD3	1:A:477:LEU:HD11	1.98	0.46
1:B:358:ILE:HD11	1:B:394:ILE:HG21	1.98	0.46
1:A:21:LYS:HB3	1:A:24:ASP:OD1	2.15	0.46
1:B:394:ILE:HD13	1:B:397:GLN:NE2	2.30	0.46
1:B:109:LYS:HA	1:B:112:LEU:CD2	2.46	0.46
1:A:239:ILE:HD13	1:A:249:GLN:NE2	2.31	0.45
1:A:372:ASN:HD22	1:A:375:GLY:N	2.09	0.45
1:B:282:ASP:OD1	1:B:373:HIS:ND1	2.48	0.45
1:A:255:VAL:HG11	1:A:330:LEU:HD21	1.99	0.45
1:B:143:TYR:HA	1:B:289:ARG:HH22	1.81	0.45
1:B:111:GLN:HB3	1:B:135:THR:HG22	1.99	0.45
1:B:346:ILE:O	1:B:365:VAL:HB	2.17	0.45
1:A:75:ILE:HD11	4:A:560:HEM:HAB	1.98	0.44
1:B:122:ILE:HG21	1:B:128:PHE:CZ	2.52	0.44
1:B:388:LEU:HD22	1:B:392:MET:HG2	1.98	0.44
1:B:244:SER:O	1:B:246:LYS:N	2.50	0.44
1:B:467:VAL:HG11	1:B:477:LEU:HD21	1.98	0.44
1:A:400:LEU:HA	1:A:403:LYS:HD3	2.00	0.44
3:B:570:FMN:H9	3:B:570:FMN:H1'2	1.55	0.44
1:B:201:LYS:HE3	1:B:233:CYS:SG	2.57	0.44
1:B:196:ALA:HB2	1:B:226:MET:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:MET:CE	1:B:250:TRP:HH2	2.31	0.44
1:A:20:ASN:HB3	1:A:55:GLY:HA3	2.00	0.44
1:B:175:ARG:NH1	1:B:176:LYS:HE2	2.33	0.44
1:A:27:VAL:CG1	1:A:36:LEU:HD22	2.46	0.43
1:A:129:GLU:HG2	1:A:437:TYR:CD2	2.53	0.43
1:A:22:PRO:HG3	1:A:51:LYS:HG3	1.99	0.43
1:A:28:VAL:HG21	1:A:84:LEU:HD22	2.01	0.43
1:A:159:ASN:HB3	1:B:488:VAL:HG11	1.99	0.43
1:A:107:ALA:O	1:A:110:GLU:HG3	2.18	0.43
1:B:358:ILE:HD11	1:B:394:ILE:CG2	2.49	0.43
1:B:116:LEU:HB3	1:B:442:TYR:OH	2.19	0.43
1:A:49:VAL:HG11	4:A:560:HEM:HMD2	2.01	0.43
1:B:175:ARG:HH12	1:B:176:LYS:HE2	1.84	0.43
1:B:178:ASP:O	1:B:469:SER:HA	2.19	0.43
1:A:256:ASN:HD22	1:A:257:SER:H	1.67	0.42
1:A:508:PHE:CE2	1:B:116:LEU:HD23	2.54	0.42
1:B:175:ARG:HD2	1:B:175:ARG:HH11	1.70	0.42
1:A:276:ALA:HA	1:A:345:PRO:HD2	2.01	0.42
1:A:192:PHE:HA	1:A:429:VAL:O	2.18	0.42
1:A:396:GLU:HG3	1:A:401:LYS:CG	2.48	0.42
1:B:356:ASP:HA	1:B:359:LYS:HD2	2.02	0.42
1:B:119:LEU:HD22	1:B:449:LYS:HG2	2.02	0.42
1:A:230:LEU:HG	4:A:560:HEM:HAA2	2.02	0.42
1:B:358:ILE:HD13	1:B:398:ARG:NH1	2.35	0.42
1:B:248:ILE:HD13	1:B:248:ILE:HG21	1.73	0.42
1:B:124:ASN:HD22	1:B:126:TYR:N	2.17	0.42
1:B:382:ARG:NH2	1:B:390:GLU:OE1	2.53	0.42
1:B:146:SER:HB3	1:B:289:ARG:HB3	2.01	0.41
1:A:218:GLN:HE22	1:A:444:ARG:HH11	1.68	0.41
1:A:79:LYS:HB3	1:A:79:LYS:HE3	1.89	0.41
1:A:11:ILE:H	1:A:85:GLN:HG3	1.85	0.41
1:A:106:ILE:HD13	1:A:106:ILE:HA	1.89	0.41
1:A:175:ARG:HB2	1:A:175:ARG:HH11	1.86	0.41
1:A:40:LEU:O	1:A:47:GLN:HB3	2.20	0.41
1:B:276:ALA:HA	1:B:345:PRO:HD2	2.01	0.41
1:B:253:LEU:HD22	1:B:277:LEU:HD13	2.02	0.41
1:A:25:CYS:SG	1:A:54:ALA:CB	3.07	0.41
1:A:196:ALA:HB2	1:A:226:MET:HG2	2.02	0.41
1:B:229:THR:OG1	1:B:253:LEU:HA	2.21	0.41
1:B:102:THR:O	1:B:104:GLU:N	2.54	0.41
1:B:335:ILE:CG2	1:B:363:ILE:HD11	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:VAL:HG12	1:A:190:VAL:H	1.87	0.40
1:A:113:LYS:HE2	1:A:113:LYS:HB3	1.89	0.40
1:B:156:GLU:OE2	1:B:163:ARG:NH2	2.54	0.40
1:B:179:ILE:CD1	1:B:190:VAL:HG12	2.52	0.40
3:A:570:FMN:H9	3:A:570:FMN:H1'2	1.62	0.40
1:B:256:ASN:HD22	1:B:258:ASP:H	1.67	0.40
1:B:196:ALA:HB1	1:B:228:SER:HB2	2.01	0.40
1:B:214:ARG:HA	1:B:243:PRO:CD	2.51	0.40
1:A:139:GLN:HG3	1:A:202:LEU:HD22	2.03	0.40
1:B:418:VAL:HG11	1:B:458:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	478/506 (94%)	440 (92%)	29 (6%)	9 (2%)	10	19
1	B	383/506 (76%)	341 (89%)	34 (9%)	8 (2%)	9	16
All	All	861/1012 (85%)	781 (91%)	63 (7%)	17 (2%)	9	18

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	245	ASP
1	A	46	GLY
1	A	114	SER
1	B	103	LYS
1	B	473	LEU
1	A	24	ASP
1	A	104	GLU
1	A	298	SER

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Mol	Chain	Res	Type
1	B	146	SER
1	B	508	PHE
1	A	16	VAL
1	B	200	CYS
1	A	102	THR
1	B	242	ALA
1	A	399	ASN
1	B	105	ASP
1	A	22	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	412/435 (95%)	358 (87%)	54 (13%)	5	9
1	B	333/435 (77%)	283 (85%)	50 (15%)	3	6
All	All	745/870 (86%)	641 (86%)	104 (14%)	4	7

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	13	PRO
1	A	19	HIS
1	A	21	LYS
1	A	22	PRO
1	A	36	LEU
1	A	38	ARG
1	A	78	GLU
1	A	81	LEU
1	A	95	PRO
1	A	102	THR
1	A	110	GLU
1	A	120	ASP
1	A	124	ASN

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Mol	Chain	Res	Type
1	A	125	LEU
1	A	131	LEU
1	A	137	THR
1	A	139	GLN
1	A	152	VAL
1	A	162	HIS
1	A	169	LYS
1	A	170	ILE
1	A	175	ARG
1	A	190	VAL
1	A	206	LEU
1	A	212	VAL
1	A	236	GLU
1	A	245	ASP
1	A	255	VAL
1	A	256	ASN
1	A	259	ARG
1	A	265	LEU
1	A	323	SER
1	A	335	ILE
1	A	338	LEU
1	A	343	LYS
1	A	365	VAL
1	A	366	SER
1	A	368	VAL
1	A	372	ASN
1	A	378	LEU
1	A	388	LEU
1	A	399	ASN
1	A	402	ASP
1	A	433	ARG
1	A	444	ARG
1	A	448	GLU
1	A	460	MET
1	A	464	LEU
1	A	477	LEU
1	A	483	LEU
1	A	484	LYS
1	A	490	VAL
1	A	492	ASN
1	B	105	ASP
1	B	108	ARG

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Mol	Chain	Res	Type
1	B	110	GLU
1	B	112	LEU
1	B	124	ASN
1	B	131	LEU
1	B	136	LEU
1	B	139	GLN
1	B	152	VAL
1	B	162	HIS
1	B	163	ARG
1	B	186	SER
1	B	209	GLU
1	B	222	LYS
1	B	230	LEU
1	B	244	SER
1	B	248	ILE
1	B	252	GLN
1	B	255	VAL
1	B	256	ASN
1	B	275	LYS
1	B	277	LEU
1	B	286	LEU
1	B	292	ASP
1	B	295	LEU
1	B	325	PHE
1	B	329	SER
1	B	338	LEU
1	B	343	LYS
1	B	353	ARG
1	B	365	VAL
1	B	368	VAL
1	B	376	ARG
1	B	378	LEU
1	B	379	ASP
1	B	384	PRO
1	B	388	LEU
1	B	397	GLN
1	B	399	ASN
1	B	404	LEU
1	B	408	VAL
1	B	444	ARG
1	B	464	LEU
1	B	465	LEU

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Mol	Chain	Res	Type
1	B	477	LEU
1	B	483	LEU
1	B	484	LYS
1	B	492	ASN
1	B	501	GLU
1	B	509	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	124	ASN
1	A	157	ASN
1	A	162	HIS
1	A	204	ASN
1	A	218	GLN
1	A	225	GLN
1	A	249	GLN
1	A	252	GLN
1	A	256	ASN
1	A	288	GLN
1	A	372	ASN
1	A	377	GLN
1	A	439	ASN
1	A	497	ASN
1	B	124	ASN
1	B	162	HIS
1	B	218	GLN
1	B	247	GLN
1	B	252	GLN
1	B	256	ASN
1	B	377	GLN
1	B	397	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	HEM	A	560	1	24,50,50	1.89	5 (20%)	16,82,82	1.70	4 (25%)
3	FMN	A	570	2	32,33,33	2.66	9 (28%)	34,50,50	2.97	11 (32%)
2	SO3	A	580	3	1,3,3	0.82	0	0,3,3	0.00	-
3	FMN	B	570	2	32,33,33	2.27	7 (21%)	34,50,50	3.29	13 (38%)
2	SO3	B	580	3	1,3,3	0.71	0	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	A	560	1	-	0/6/54/54	0/0/8/8
3	FMN	A	570	2	2/2/4/4	0/18/18/18	0/3/3/3
2	SO3	A	580	3	-	0/0/0/0	0/0/0/0
3	FMN	B	570	2	2/2/4/4	0/18/18/18	0/3/3/3
2	SO3	B	580	3	-	0/0/0/0	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	570	FMN	C1'-N10	-12.06	1.35	1.48
3	B	570	FMN	C1'-N10	-10.35	1.37	1.48
4	A	560	HEM	C3C-C2C	-4.59	1.34	1.40
4	A	560	HEM	C3C-CAC	-4.11	1.38	1.47
4	A	560	HEM	C3B-C2B	-3.89	1.35	1.40
4	A	560	HEM	C3B-CAB	-3.87	1.39	1.47
3	A	570	FMN	C7M-C7	-3.23	1.44	1.51
3	B	570	FMN	C6-C5A	-3.07	1.37	1.41
3	A	570	FMN	C6-C5A	-2.88	1.37	1.41
3	B	570	FMN	C2'-C3'	-2.64	1.48	1.53
3	A	570	FMN	C4A-C10	-2.58	1.36	1.40
3	A	570	FMN	O4'-C4'	-2.34	1.38	1.43
3	B	570	FMN	C9A-C5A	-2.21	1.37	1.42
3	A	570	FMN	P-O2P	-2.13	1.47	1.54
3	A	570	FMN	C9A-C5A	-2.03	1.38	1.42
3	B	570	FMN	C9-C9A	-2.02	1.36	1.40
3	A	570	FMN	C4-C4A	2.01	1.45	1.41
3	B	570	FMN	C4-N3	2.11	1.36	1.33
3	B	570	FMN	C4-C4A	2.17	1.45	1.41
4	A	560	HEM	CBB-CAB	2.40	1.46	1.28
3	A	570	FMN	C4-N3	2.76	1.38	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	570	FMN	C4A-C4-N3	-7.73	113.41	123.52
3	A	570	FMN	N3-C2-N1	-7.15	115.65	127.69
3	A	570	FMN	C4A-C4-N3	-6.03	115.64	123.52
3	B	570	FMN	N3-C2-N1	-5.61	118.25	127.69
3	B	570	FMN	C4-C4A-N5	-4.02	113.81	118.70
3	A	570	FMN	O5'-P-O1P	-3.54	98.18	107.08
3	B	570	FMN	O2P-P-O5'	-2.69	98.87	106.72
4	A	560	HEM	CMD-C2D-C1D	-2.10	124.73	128.31
3	A	570	FMN	O3'-C3'-C4'	2.01	113.93	108.73
4	A	560	HEM	C3B-C4B-NB	2.02	111.82	109.21
3	A	570	FMN	O2P-P-O1P	2.05	117.33	110.63
3	B	570	FMN	O3P-P-O2P	2.10	115.17	107.44
3	A	570	FMN	C1'-C2'-C3'	2.42	116.75	109.82
4	A	560	HEM	CBD-CAD-C3D	2.46	116.79	112.47
3	B	570	FMN	C1'-C2'-C3'	2.81	117.84	109.82
3	A	570	FMN	O4'-C4'-C3'	2.92	116.48	108.96
3	A	570	FMN	C4A-N5-C5A	3.35	120.67	116.72
3	B	570	FMN	O4'-C4'-C5'	3.54	117.81	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	570	FMN	O3'-C3'-C4'	3.62	118.12	108.73
3	B	570	FMN	C5A-C9A-N10	3.75	120.39	117.58
3	B	570	FMN	O4'-C4'-C3'	4.09	119.49	108.96
3	A	570	FMN	O2'-C2'-C1'	4.26	120.46	109.93
4	A	560	HEM	CAA-CBA-CGA	4.28	121.11	112.78
3	B	570	FMN	O2'-C2'-C1'	4.63	121.38	109.93
3	A	570	FMN	C4-C4A-C10	7.62	124.82	119.94
3	B	570	FMN	C4-N3-C2	8.16	121.96	115.16
3	A	570	FMN	C4-N3-C2	8.29	122.08	115.16
3	B	570	FMN	C4-C4A-C10	9.44	125.98	119.94

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	570	FMN	C4'
3	B	570	FMN	C2'
3	A	570	FMN	C4'
3	A	570	FMN	C2'

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	560	HEM	5	0
3	A	570	FMN	1	0
3	B	570	FMN	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.